

Variational Approach to Localization Length for Two-Dimensional Hubbard Model

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As a measure to ascertain whether a system is metallic or insulating, localization length λ_N , which represents the spread of electron distribution, can be a useful quantity, especially for approaching a metal-insulator transition from the insulator side. We try to calculate λ_N using a variational Monte Carlo method for normal (paramagnetic), superconducting and antiferromagnetic states in the square-lattice Hubbard model. It is found that the behavior of λ_N is consistent with what is expected from other quantities, and gives information complementary to another measure, the Drude weight.

KEYWORDS: metal-insulator transition, localization length, Drude weight, variational Monte Carlo method, Hubbard model

1. Introduction

Because, in many strongly correlated electron systems, itinerancy and localization of conduction electrons are vital to their properties, appropriate and convenient measures to determine whether the system is a metal or an insulator have been pursued for long years. Various physical quantities are available to consider metal-insulator transitions, such as quasi-particle renormalization factor Z , charge structure factor $N(\mathbf{q})$, chemical potential μ and the Drude weight D , DC component of conductivity, introduced by Kohn [1, 2]. Because these quantities are obtained within ground states, the nature of being a metal or an insulator is already inherent in the ground-state wave functions. Correctly, $N(\mathbf{q})$ and μ are not measures, and the vanishing of Z do not necessarily indicate an insulator, but represent a gap opening in some degree of freedom. Actually, Z do not distinguish an s -wave superconducting (SC) state (gapped in the spin sector, but gapless in the charge sector) from an insulating state (gapped in the charge sector). As for μ [3], we have to find a jump as a function of electron density n ($= N/N_s$; N : electron number, N_s : site number) or doping rate δ ($= 1 - n$), in addition to differentiating the total energy with respect to n . It is a little laborious. Here, we are interested in strongly correlated systems, for which a variational Monte Carlo (VMC) method [4] is very useful for its exact treatment of local electron correlation without a minus sign problem. Thus, in this work, we discuss useful measures of metal-insulator transitions for VMC calculations, namely, D and in particular localization length λ_N . We adopt a Hubbard model on the square lattice, which is a plausible model of the cuprate superconductors, and undergoes a Mott transition at half filling at $U \sim W$ (band width), unless an antiferromagnetic (AF) order is assumed.

Since the discovery of cuprate superconductors, D has been intensively studied, because D is directly obtained from experiments; in particular, anomalous δ dependence of superfluid density ρ_s [5], which is equivalent to D in SC states [2], in cuprates is regarded as indubitable evidence of a doped Mott insulator. To obtain D in the two-dimensional Hubbard model, we have to calculate the

ground-state energy of the Hamiltonian [6],

$$\mathcal{H}(\mathbf{A}) = -t \sum_{\langle i,j \rangle, \sigma} \left[e^{i\mathbf{A} \cdot (\mathbf{r}_i - \mathbf{r}_j)} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right] + U \sum_j n_{j\uparrow} n_{j\downarrow}, \quad (1)$$

where $c_{j\sigma}(c_{j\sigma}^\dagger)$ is the electron annihilation (creation) operator of spin σ at site j , $n_{j\sigma} = c_{j\sigma}^\dagger c_{j\sigma}$, t (hopping integral) and U (onsite interaction) are positive variables, and \mathbf{A} is a virtual vector potential. D is given by $D = d^2 E(\mathbf{A})/dA^2$ with $E(\mathbf{A}) = \langle \mathcal{H}(\mathbf{A}) \rangle$. If the system is metallic (insulating), D is finite (vanishes). In variation theories, however, a metal-insulator transition had not been described by means of D until recently [7], namely, D remained positive finite in insulating states even if binding factors between a doubly occupied site (doublon) and an empty site (holon) [8] are introduced, with which Mott transitions are definitely described in terms of other quantities. Recently, this problem was solved as far as the range of $U \gtrsim U_c$ (U_c/t : Mott transition point) is concerned [6]. The ground state of eq. (1) must be essentially complex, because the matrix elements are complex owing to the Peierls phase $e^{i\mathbf{A} \cdot (\mathbf{r}_i - \mathbf{r}_j)}$. Therefore, an appropriate wave function should have a configuration-dependent phase factor \mathcal{P}_θ [6]. Thereby, not only Mott transitions are clearly identified by D , but linear behavior of $\rho_s(\delta)$ (Uemura plot) [5] is obtained. We now know that this type of phase factors are indispensable for addressing current-carrying states such as various flux states [9] for intermediate and strong correlations. On the other hand, for insulators in weakly correlated regimes such as Slater-type AF insulators, we found that appropriate trial wave functions for finite \mathbf{A} should consist of multiple determinants; it seems technically difficult to treat them with the present VMC scheme [6]. In calculating D , fine tuning of the trial functions seems necessary according to individual cases.

Although D gives useful information in a metallic regime, D does not tell how rigidly electrons are bound in an insulating regime, where D always vanishes. As an alternative measure of metal-insulator transition from the insulator side, Resta [10, 11] introduced localization length λ_N , which approaches the spread of the electronic distribution, $\sqrt{[\langle (\sum_j x_j)^2 \rangle - \langle \sum_j x_j \rangle^2]/N}$, as the system size increases. λ_N represents how electrons can broaden in an insulating state; we can judge that the system is insulating (metallic), if λ_N remains finite (diverges) as the system size is increased to infinity. Thus, a Mott transition point can be determined by the diverging point of λ_N , without carrying out differentiating operations in contrast to D . In early studies for one-dimensional systems, λ_N or a corresponding susceptibility was calculated using exact diagonalization [11], quantum Monte Carlo method [12], and density matrix renormalization group [13]. Regarding VMC, λ_N was calculated for a hydrogen chain [14]; it seems that λ_N can be a good measure.

In the following, we calculate the localization length in a Hubbard model on the square lattice [eq. (1) with $\mathbf{A} = \mathbf{0}$] using a VMC method, to confirm that λ_N is an appropriate measure of a Mott transition. In sec. 2, we describe the method used in this study. In sec. 3, we show results of λ_N , and have discussions. A conclusion is given in sec. 4.

2. Method

In this section, we briefly explain variational wave functions used and the localization length λ_N . We study λ_N with three types of wave functions: (i) a $d_{x^2-y^2}$ -wave superconducting (SC) or singlet-pairing state Ψ_{SC} , (ii) a paramagnetic or normal state Ψ_{N} , and (iii) an AF state Ψ_{AF} . Because these functions are applied to a highly correlated Hamiltonian, we adopt short-range Jastrow-type wave functions, which are composed of two parts: $\Psi = \mathcal{P}\Phi$. Here, Φ represents a one-body wave function, $\Phi = \Phi_{\text{SC}}$, Φ_{N} or Φ_{AF} , each of which is a solution of the Hartree-Fock approximation without imposing the SCF condition. They are explicitly written as,

$$\Phi_{\text{SC}} = \left(\sum_{\mathbf{k}} a_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \right)^{N/2} |0\rangle, \quad a_{\mathbf{k}} = \frac{\Delta_d(\mathbf{k})}{\epsilon_{\mathbf{k}} - \zeta + \sqrt{(\epsilon_{\mathbf{k}} - \zeta)^2 + |\Delta_d(\mathbf{k})|^2}}, \quad (2)$$

$$\Phi_N = \prod_{k \in \text{FS}, \sigma} c_{k\sigma}^\dagger |0\rangle, \quad (\text{FS: Fermi sea}) \quad (3)$$

$$\Phi_{\text{AF}} = \prod_{\mathbf{k}, \sigma} (\alpha_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger + \tilde{\sigma} \beta_{\mathbf{k}} c_{\mathbf{k}+\mathbf{Q}\sigma}^\dagger) |0\rangle, \quad \alpha_{\mathbf{k}}(\beta_{\mathbf{k}}) = \sqrt{\frac{1}{2} \left(1 - (+) \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\text{AF}}^2}} \right)}. \quad (4)$$

In d -wave BCS wave function Φ_{SC} , $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$, ζ is a variational parameter corresponding to the chemical potential in the limit of $U/t \rightarrow 0$, and the pair potential is assumed as $\Delta_d(\mathbf{k}) = \Delta(\cos k_x - \cos k_y)$ with Δ being a variational parameter. In Φ_{AF} , $\tilde{\sigma} = \pm 1$ according to $\sigma = \uparrow$ or \downarrow , $\mathbf{Q} = (\pi, \pi)$, and Δ_{AF} is a variational parameter related to the staggered moment. As for the many-body part \mathcal{P} in Ψ , we consider only dominant factors, $\mathcal{P} = \mathcal{P}_G \mathcal{P}_Q$, in common for the three Ψ 's. The most fundamental one is the onsite (Gutzwiller) factor, $\mathcal{P}_G = \prod_j [1 - (1-g)n_{j\uparrow}n_{j\downarrow}]$ with g being a variational parameter ($0 \leq g \leq 1$). The second factor is a doublon-holon binding factor between nearest-neighbor (NN) sites [8], which is indispensable for inducing a Mott transition: $\mathcal{P}_Q = \prod_j [1 - \mu_1 Q_j^1] \prod_i [1 - \mu_2 Q_i^2]$, with $Q_j^1 = n_{j\uparrow}n_{j\downarrow} \prod_{\tau} [1 - (1 - n_{j+\tau\uparrow})(1 - n_{j+\tau\downarrow})]$, and $Q_j^2 = (1 - n_{j\uparrow})(1 - n_{j\downarrow}) \prod_{\tau} (1 - n_{j+\tau\uparrow}n_{j+\tau\downarrow})$. Here, μ_1 and μ_2 are variational parameters ($0 \leq \mu_1, \mu_2 \leq 1$), and τ runs over the NN sites of site j . Some properties of these wave functions when applied to eq. (1) are known [6, 15–17]. At half filling, it was confirmed through the behavior of Z , $N(\mathbf{q})$, D , etc. that Ψ_{SC} and Ψ_N exhibit first-order Mott transitions at $U/t \sim 6.5$ and 8.5 , respectively. On the other hand, it is expected that an AF state becomes the ground state and insulating for any $U/t (> 0)$ without transitions. Actually, Ψ_{AF} is insulating and has the lowest energy among the three Ψ 's for $U/t \gtrsim 1.5$. For $0 < U/t \lesssim 1.5$, the AF order seems to vanish in Ψ_{AF} , but this is irrelevant to the following discussions. In less-than-half-filled cases, the three Ψ 's are always metallic.

In an insulator (metal), the ground-state wave function is localized (delocalized). In a system under the periodic boundary condition, localization can be treated in parallel with the modern theory of polarization [10, 11]. The degree of localization is embedded in a complex number z_N defined below, whose modulus is the definition of localization length λ_N :

$$\lambda_N = \left(\frac{L}{2\pi} \right) \sqrt{-\frac{\ln |z_N|^2}{N}} \quad \text{with} \quad z_N = \langle \Psi | e^{i\frac{2\pi}{L}X} | \Psi \rangle \quad (L \rightarrow \infty), \quad (5)$$

where L is the system size in one (x) direction, and X is the sum of x coordinates of electrons: $X = \sum_{j,\sigma} x_j n_{j\sigma}$. If we expand z_N with respect to $2\pi/L$ and substitute it in the expression of λ_N in eq. (5), the definition of localization length, $\sqrt{(\langle X^2 \rangle - \langle X \rangle^2)/N}$, is obtained as the leading term. Therefore, we should check L dependence of λ_N to monitor the deviation owing to higher-order terms. When the state is extremely localized like a δ function, z_N becomes 1; z_N is finite ($0 < |z_N| < 1$) for general localized states, whereas z_N vanishes when the state is delocalized. Equivalently, λ_N converges to a finite value for an insulator, but diverges as L increases for a metallic system. Using the above wave functions, the expectation value of z_N is easily calculated by VMC.

We carry out a series of VMC calculations to estimate z_N using correlated measurement with quasi-Newton algorithm for large systems of $L \times L$ sites ($L = 12\text{--}20$). A typical sample number in this study is $M = 2.4 \times 10^5$.

3. Results

Let us start with U/t dependence of $|z_N|$ at half filling. In Fig. 1(a), we plot $|z_N|$ obtained by VMC calculations for the three states. For Ψ_{SC} , $|z_N|$ is almost zero for $U/t \leq 6$, but suddenly increases with a jump at approximately $U/t = 6.5$, and tends to unity for $U/t \geq 7$. As mentioned above, this behavior of $|z_N|$ indicates that the system is conductive (insulating) for $U/t < 6.5$ ($U/t > 6.5$), and at $U/t = 6.5$

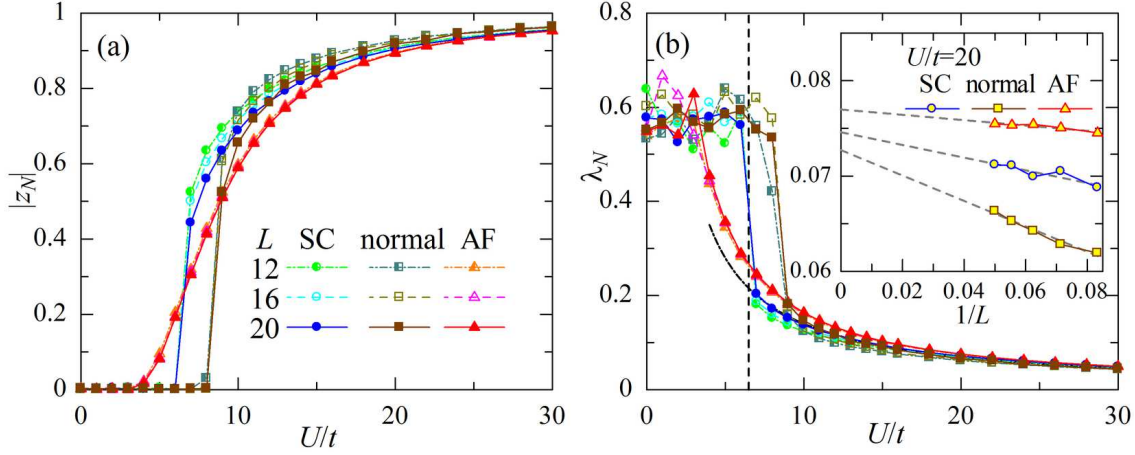


Fig. 1. (Color online) (a) Absolute values of z_N are shown for the three Ψ 's as a function of U/t at half filling for three L 's. (b) Localization length are compared among the three wave functions. The symbols are common to (a). A dash-dotted curve of $\propto t/U$ is added as a guide for eyes. The vertical dashed line indicates the metal-insulator transition point of Ψ_{SC} . Inset in (b) shows the extrapolation of λ_N to $L \rightarrow \infty$ for the three states for $U/t = 20$ from the data for $L = 12$ -20. The number of samples is 2.4×10^5 .

a sharp (first-order-like) SC-insulator transition arises. This result is quantitatively consistent with that of the previous studies [6, 15, 16], in which this Mott transition was confirmed by various quantities such as a SC pairing correlation function and the Drude weight. The behavior of $|z_N|$ of Ψ_N is similar to that of Ψ_{SC} except for the Mott transition point, and is consistent with that of the previous results. Although appreciable system-size dependence in $|z_N|$ is observed both for Ψ_{SC} and Ψ_N , especially near the transition points, they will not qualitatively change the features of Mott transition. We will return to this point again in connection with λ_N . $|z_N|$ of Ψ_{AF} is again almost zero for $0 < U/t \leq 3$, but this time $|z_N|$ increases smoothly for $U/t > 3$, as U/t increases, without anomalous behavior like a jump. Thus, Ψ_{AF} is insulating at least for $U/t > 3$. Considering Ψ_{AF} is insulating for more smaller values of U/t , we expect that the value of $|z_N|$ is very small but still non zero for $U/t < 3$. In this range, it is difficult to determine the accurate behavior of $|z_N|$, because statistical errors in VMC exceed the magnitude of $|z_N|$. We will discuss this point later again. The system-size dependence for Ψ_{AF} is by far smaller than those for Ψ_{SC} and Ψ_N .

We turn to the localization length λ_N , which is calculated from z_N through eq. (5). In Fig. 1(b), we plot λ_N obtained from the data in Fig. 1(a). As a whole, λ_N tends to decrease as U/t increases; this behavior agrees with our intuition that the electrons are more localized as the repulsive interaction becomes stronger. Corresponding to the behavior of $|z_N|$, λ_N for Ψ_{SC} and Ψ_N exhibit discontinuities at $U/t = 6.5$ and 8.5 , respectively; λ_N of Ψ_{AF} is smooth for $U/t \gtrsim 3$.

First, we discuss the insulating regimes. Here, each λ_N decreases approximately as a function of t/U ($= J/4t$), indicating that the insulating regime is effectively described by an AF Heisenberg model with the exchange coupling $\sim J$, which is the sole energy scale. Now, we look at the system-size dependence. In the inset of Fig. 1, we plot λ_N at $U/t = 20$ in the insulating regime as a function of $1/L$. The system-size dependence is the largest in Ψ_N and the smallest in Ψ_{AF} , but the order among the three does not seem to change in the limit of $L \rightarrow \infty$. The localization length of Ψ_{SC} is a little longer than that of Ψ_N , indicating electrons in SC is more mobile than in the normal state even in a insulating regime. This corresponds to the fact that the kinetic energy is lower for Ψ_{SC} than for Ψ_N (not shown), namely, a kinetic-energy-driven SC ($\Psi_N \rightarrow \Psi_{SC}$) transition is realized, as previous studies showed [15]. Incidentally, for smaller values of U/t ($U_c < U < 20t$), we cannot implement reliable extrapolations for Ψ_{SC} and especially Ψ_N , because the system-size dependence

of λ_N becomes somewhat irregular. It seems that this is not only owing to the sampling errors but to the short range nature of the trial wave functions. It is possible that a long-range correlation factor is necessary for systems of large λ_N to stably estimate λ_N near Mott transitions. The notion of a kinetic-energy-driven transition is similarly applicable to the AF transition ($\Psi_N \rightarrow \Psi_{AF}$), because $\lambda_N^{AF} > \lambda_N^N$. The reason λ_N^{AF} is the largest is that electrons are more likely to hop to NN sites owing to the spin alternate configurations in Ψ_{AF} .

Next, we consider the results of λ_N in weakly correlated regimes. In the insulating regimes discussed above, the expectation values of λ_N converges at finite values, as expected. On the other hand, in weakly correlated regimes ($U < U_c$ for Ψ_{SC} and Ψ_N ; $U \lesssim 3t$ for Ψ_{AF}), λ_N does not diverge as $L \rightarrow \infty$, but has scattered values around 0.6 irrespective of the system size, as found in Fig. 1(b). An origin of this result probably lies in the statistical errors in VMC sampling. The expectation values of $|z_N|$ for these correlation strengths are extremely close to zero but positive finite. Therefore, if the numerical error ϵ exceeds the correct expectation value, the estimation by VMC yields an arbitrary value of order ϵ as $|z_N|$. To verify this possibility, we carry out a series of VMC calculations for Ψ_{SC} by widely varying the sampling number M for a fixed $L (= 12)$; the statistical errors are proportional to $1/\sqrt{M}$. The results are plotted in Fig. 2(a). We find that the value of λ_N steadily increases as M increases, although the increments are small because λ_N is a logarithmic function of $|z_N|$ [eq. (5)]. Thus, in order to estimate λ_N accurately for a system with large λ_N , it is necessary to precisely determine $|z_N|$ of a large negative power. In this connection, we calculate λ_N for less-than-half-filled or doped systems, which are metallic for any value of U/t , with the same sample number as in Fig. 1(b). As shown in Fig. 2(b), the results are scattered around $\lambda_N = 0.6$ in broad accordance with that for the weakly interacted half-filled case in Fig. 1(b). We can perceive a slight tendency for λ_N to increase as electron density (n) decreases. Anyway, the present VMC calculations yield a reliable value of λ_N for an insulator of $\lambda_N \lesssim 0.5$.

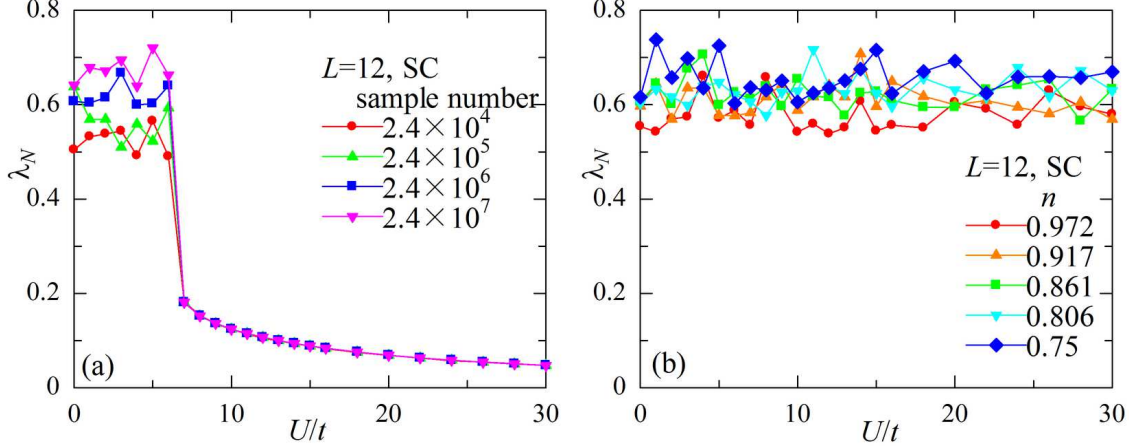


Fig. 2. (Color online) (a) Expectation values of localization length at half filling are compared for different sample numbers in the VMC calculations for Ψ_{SC} . (b) Localization length estimated with the same VMC procedure for several doped systems. n indicates an electron density. The number of sample is 2.4×10^5 .

Finally, we touch on λ_N of Ψ_{AF} . Judging from other quantities, Ψ_{AF} is insulating at least for $U/t \gtrsim 1.5$, as mentioned. Therefore, λ_N should converge at finite values in this range. Correspondingly, λ_N in Fig. 1(b) exhibits a smooth converged curve for large values of U/t down to $U/t \sim 3$. However, at $U/t = 3$, λ_N reaches 0.6 still in the insulating phase. Thus, to address an insulator in weak-correlation regimes, a formalism or an algorithm in a new line seems necessary.

4. Summary

Localization length λ_N , which is the variance in coordinates of electrons, is calculated for the two-dimensional Hubbard model to distinguish a metal from an insulator, using a variational Monte Carlo method. λ_N thus obtained definitely indicates a Mott transition point (U_c) by a discontinuity for a normal or a d -wave pairing state, whose U_c is at a correlation strength broadly of the band width. On the other hand, we found that reliable estimation of λ_N by VMC is not easy for a system of λ_N beyond a threshold value determined by the numerical errors (~ 0.6 in the present setting), regardless of being a metal or an insulator. Therefore, the present scheme is not necessarily suitable to address weakly correlated insulators such as a Slater-type antiferromagnetic insulator. Nevertheless, we may say that λ_N is a useful quantity to discuss Mott transitions using various Monte Carlo methods.

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